Homework for IMI Glass Processing Course, Lectures Feb. 12 and 17, 2015:

1. Sol-gel precursors undergo chemical reactions with water and with each other. To predict these reactions, one approach is the *Partial Charge Model*, based on electronegativities. The model predicts electrical interactions between the atoms or ions in the molecule. The electronegativity of the <u>complex</u> X(C) is calculated according to:

$$X(C) = \frac{\sqrt{X_{Si}^{\circ}} + N\sqrt{X_{O}^{\circ}} + (2N-h)\sqrt{X_{H}^{\circ}} + 1.36(z-h)}{\frac{1}{\sqrt{X_{Si}^{\circ}}} + \frac{N}{\sqrt{X_{O}^{\circ}}} + \frac{2N-h}{\sqrt{X_{H}^{\circ}}}}$$

and the partial charge δ_{Si} is calculated according to:

$$\delta_{Si} = \frac{X(C) - X_{Si}^{\circ}}{1.36\sqrt{X_{Si}^{\circ}}}$$

a. Using the electronegativities below and the values for **N** (coordination number = **4**), **z** (valence/formal charge of Si = **4**) and **h** (number of hydroxo ligands), calculate X(C) for the following *complex* under basic conditions, where h = **5**:

$[SiO(OH)_3]^-$ $\quad\quad$ X(C) = __________

b. Calculate the partial charge on Si, δ_{Si}, for the *complex*.

$[SiO(OH)_3]^-$ $\quad\quad$ δ_{Si} = __________

c. If the partial charge on Si is > 0.3 the *complex* can dimerize (a polymer of 2 units) by condensation. Is this possible? (Yes or No)

$$2[SiO(OH)_3]^- \rightarrow [Si_2O_4(OH)_3]^{3-} + H_2O$$

H 2.10																	He 3.20
Li 0.97	Be 1.57											B 2.02	C 2.50	N 3.07	O 3.50	F 4.10	Ne 5.10
Na 1.01	Mg 1.29											Al 1.47	Si 1.74	P 2.11	S 2.48	Cl 2.83	Ar 5.10
K 0.91	Ca 1.04	Sc 1.23	Ti 1.32	V 1.56	Cr 1.59	Mn 1.63	Fe 1.72	Co 1.75	Ni 1.80	Cu 1.75	Zn 1.66	Ga 1.82	Ge 2.00	As 2.20	Se 2.50	Br 2.69	Kr 3.10
Rb 0.89	Sr 0.99	Y 1.19	Zr 1.29	Nb 1.45	Mo 1.56	Tc 1.67	Ru 1.78	Rh 1.84	Pd 1.85	Ag 1.68	Cd 1.60	In 1.49	Sn 1.89	Sb 1.98	Te 2.15	I 2.33	Xe 2.60
Cs 0.87	Ba 0.89	Lant	Hf 1.36	Ta 1.50	W 1.59	Re 1.88	Os 1.99	Ir 2.05	Pt 2.00	Au 2.02	Hg 1.80	Tl 1.60	Pb 1.92	Bi 2.03	Po 2.12	At 2.28	Rn 2.30
Fr 0.86	Ra 0.95	Uran															
		Lant	La 1.18	Ce 1.17	Pr 1.18	Nd 1.19	Pm 1.20	Sm 1.20	Eu 1.13	Gd 1.27	Tb 1.24	Dy 1.26	Ho 1.28	Er 1.30	Tm 1.30	Yb 1.24	Lu 1.36
		Uran	Ac 1.12	Th 1.24	Pa 1.22	U 1.24	Np 1.22	Pu 1.24	Am 1.25	Cm 1.20	Bk 1.20	Cf 1.20	Es 1.20	Fm 1.20	Md 1.20	No 1.20	Lw 1.20

2. To emphasize the scaling for nanomaterials like colloidal silica:

a. Suppose we have 20 cm^3 of silica in 1 cm radius droplets. Each has a volume of ($4/3\ \pi r^3$) _______ cm^3 and a surface area of ($4\pi r^2$) _____ cm^2. As we need about ______ droplets we would have a total area of __________ cm^2.

b. The same silica is split into 0.1 cm radius droplets. Each has a volume of ($4/3\ \pi r^3$) _______ cm^3 and a surface area of ($4\pi r^2$) _____ cm^2. As we need about ______ droplets we would have a total area of __________ cm^2.

c. Finally, the same silica is split into 100 nm radius droplets or colloids. Each has a volume of ($4/3\ \pi r^3$) _______ cm^3 and a surface area of ($4\pi r^2$) _____ cm^2. As we need about ______ droplets we would have a total area of __________ cm^2.

d. Make a plot of droplet volume vs radius. Superimpose a plot of droplet area vs. radius.

e. Make a plot of surface-to-volume ratio vs. radius.

f. Make a plot of total area vs. radius.

g. What do these plots tell you about what to expect from nanomaterials?